MM5 Simulations for TexAQS 2000 Episode

Task 4: Review of the TKE PBL schemes in MM5

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Introduction

ATMET has performed numerous sensitivity simulations with MM5 for both the 1993 and 2000 episodes for the Houston-Galveston region (ATMET, 2002a; ATMET, 2003a; ATMET, 2003b). A major component of these simulations has been the testing of the various PBL schemes that are implemented in MM5. The results of these simulations consistently showed that, of all the PBL schemes in MM5, the MRF scheme usually provided the best results.

However, as many other MM5 users have noted also, the MRF scheme consistently overestimates the height of the PBL, which is crucial for good air quality simulations. Virtually all of the experiments we have conducted show this tendency to overestimate the depth of the boundary layer, especially during the daytime hours. This overestimation manifests itself in numerous was. For example, in ATMET 2003b, the too rapidly-growing daytime PBL played a role in a significant low bias of dew point temperature on many days.

The MM5 MRF PBL scheme is designed after a procedure described by Hong and Pan (1996), which followed very closely on earlier work of Troen and Mahrt (1986). Hong and Pan first implemented this scheme in the NCEP MRF model, which is the main global forecast model run at NCEP to produce the AVN forecasts (the name of the model and forecasts have recently been changed to the GFS, Global Forecasting System). It was developed with the MRF model in mind, relatively coarse horizontal resolution, vertical resolution coarser than is usually used today in mesoscale models, and a requirement that very little computer resources be used. The scheme was later implemented in MM5 by Dudhia and Hong (personal communication).

In ATMET (2003b, 2003c), we reviewed the formulation of the MRF scheme and identified several features in the implementation that could lead to this overprediction. The MRF scheme is based on the use of a profile function for the vertical exchange coefficient. Sub-grid diffusion schemes based on the O'Brien profile function date back to at least the early 1970's. While termed a "non-local" scheme by Hong and Pan, this scheme still produces an eddy exchange coefficient where the mixing is done locally (i.e., from layer to layer). The computation of the eddy viscosity coefficients is done taking into account "non-local" effects (e.g., the O'Brien profile function).

Profile-based schemes can provide an adequate result in a "classic" PBL (surface-based, well-mixed from the ground to a strong capping inversion). However, profile schemes are unable to correctly simulate features that deviate from this classic case. This is important for the Texas Gulf Coast region because of the sea breeze development. As the cooler marine air moves ashore into a deep well-mixed PBL, an internal boundary layer is developed. A profile scheme will diagnose a particular boundary layer height. Under this level, significant vertical sub-grid mixing can occur; over this level, very little mixing is done. If the scheme diagnoses the PBL height at the level of the internal, marine air boundary layer, then vertical mixing will be shut down in the remainder of the mixed layer that lies atop the marine air. If the PBL height is diagnosed at the top of the existing deep mixed layer, then the internal boundary layer will be quickly mixed out. In either case, the physical process is not represented correctly.

In theory, a TKE-based scheme (such as Mellor-Yamada) can more correctly simulate these types of "non-classic" situations. But as mentioned above, the current implementations of TKE schemes in MM5 usually provide worse results than the MRF scheme. All three of the MM5 TKE schemes tend to exhibit a significant low bias in the PBL height, along with worse overall surface statistical verification.

However, most other models (RAMS, COAMPS, ARPS, etc.) use TKE schemes almost exclusively. In our experience with RAMS, there has been little bias in the PBL depth (for example, see ATMET, 2002b). In this report, we will present the basic formulation of a TKE scheme, using the Mellor-Yamada scheme in RAMS as an example. We will then review and compare the three TKE-based schemes in MM5 to the example. We will cover other issues regarding these schemes and their implementation in MM5. Finally, we will offer our recommendations for future investigations. We recommend a review of the MM5 TKE schemes, comparison with other models' schemes, and possible modification of the MM5 schemes to allow them to work for more general situations.

Diffusion terms in an atmospheric model

The horizontal and vertical grid spacings configured in the model determine the spatial scales of prognostic field variables that can be explicitly resolved and those which cannot. Recognizing that there may be subgrid scale fluctuations of the quantities, an averaging operator is first defined. Ideally, an *ensemble* averaging operator is desirable, however, usually the averaging operators are assumed to apply spatially over a grid cell. Once the form of the operator is assumed, a Reynolds averaging procedure of the prognostic differential equations for momentum and conservative scalars is performed to partition advective transport into resolved and unresolved components.

The unresolved flux components may be expressed in terms of covariances of the form $\overline{u_i' u_j'}$ for momentum, and $\overline{u_i' \phi'}$ for scalars, where subscripts *i* and *j* denote spatial directions *[1,2,3]*, u_i is the transporting velocity component, u_j is the transported velocity component, ϕ represents the transported scalar, an overbar represents the Reynolds average, and a prime the deviation from that average.

The contribution to the tendency of the resolved variables due to turbulent transport is given by the convergence of the turbulent fluxes

$$\left(\frac{\partial u_j}{\partial t}\right)_{TURB} = \frac{\partial}{\partial x_i}\left(\overline{u_i' u_j'}\right) \tag{1}$$

and

$$\left(\frac{\partial \phi}{\partial t}\right)_{TURB} = \frac{\partial}{\partial x_i}\left(\overline{u_i^{'}\phi^{'}}\right) \qquad (2)$$

Atmospheric models generally parameterize the unresolved transport using K-theory, in which the covariances are evaluated as the product of an eddy mixing coefficient and the gradient of the transported quantity. For scalars, this parameterization takes the form

$$\overline{u_i^{'}\phi^{'}} = -K_{hi}\frac{\partial \phi}{\partial x_i} \qquad (3)$$

where K_{hi} is the eddy mixing coefficient for scalars which applies to the *i*-direction. K_{hi} is never negative, which restricts the parameterized eddy fluxes to always be down-gradient.

For velocity components, two different forms are used, depending on the scales of motion resolved by the model grid. When the horizontal grid spacing is comparable to the vertical spacing so that convective motions are resolved, the Reynolds stresses are evaluated from

$$\overline{u_i^{'}u_j^{'}} = -K_{mi}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \qquad (4)$$

which applies to the *i*-direction for *i* and *j = [1,2,3]*, where K_{mi} is the eddy mixing coefficient for momentum. In this case, it is assumed that $K_{mi} = K_{mj}$, and therefore, $\overline{u_i^{'}u_j^{'}} = \overline{u_j^{'}u_i^{'}}$.

This symmetry of the Reynolds stress components is a basic physical property of a fluid. Violation of this property in numerical models is equivalent to applying a fictitious external torque to the fluid wherever a violation occurs. In simulations where convective motions are resolvable, this may lead to significant errors in the numerical solution.

If the horizontal grid spacing is much larger than the vertical spacing (as is usually the case when performing atmospheric simulations for air quality modeling), preventing explicit representation of convective vertical motion, it is not essential that Reynolds stresses be symmetric between the vertical and a horizontal direction. The constraint imposed by low horizontal resolution in the model prevents the solution from being strongly affected by fictitious external horizontal torque. On the other hand, relatively coarse horizontal grids require a larger value of K_{mi} in the horizontal directions than in the vertical. This horizontal mixing coefficient is larger in magnitude than any physical transport by turbulent eddies, and is required purely for numerical stability. Consequently, asymmetry of the Reynolds stresses which involve the vertical direction is a practical requirement. Hence, for coarse horizontal grid spacing we apply [4] only in the horizontal directions by restricting *i* and *j* to *[1,2],* and use the following expression whenever i and/or *j* is 3,

$$\overline{u_i' u_j'} = -K_{mi}\left(\frac{\partial u_i}{\partial x_j}\right) \tag{5}$$

In RAMS, there are currently six basic options for computing K_{mi} and K_{hi}. Two of these are based on the Smagorinsky (1963) scheme which relates the mixing coefficients to the fluid strain or deformation rate, and include corrections for the influence of Brunt-Vaisala frequency (Hill, 1974) and Richardson number (Lilly, 1962). These are purely local schemes in which the mixing coefficients depend only on the local and current flow properties. The other four options diagnose mixing coefficients from a parameterized subgrid-scale turbulent kinetic energy (TKE) which is prognosed in the model. Although the diagnosis is based on the local current value of TKE, these schemes can be regarded as non-local because the TKE can be generated elsewhere in the domain and transported to new locations.

Of the two local schemes, and of the two TKE schemes, three apply in cases of small horizontal grid spacing where [4] is used, and the other applies with large horizontal grid spacing where [5] is used. This latter scheme is based from the Mellor and Yamada (1974, 1982) scheme and will be described in the next section.

An example of the Mellor-Yamada TKE scheme

We now consider an example implementation of the Mellor-Yamada (1974, 1982) (hereinafter, MY) scheme where prognostic TKE is used to evaluate eddy mixing coefficients. If the horizontal grid spacing is large, the MY scheme is used to compute the vertical mixing coefficients, while the local deformational scheme described above is used for horizontal mixing. The MY scheme is an ensemble closure, which assumes that the Reynold's-averaged flow cannot resolve convection so that parameterized convection performs all vertical transport.

The technique developed by MY is a so-called level 2.5 scheme. It has also been termed an order 1.5 scheme. In RAMS, we have implemented modifications for the case of growing turbulence (Helfand and Labraga, 1988). The fields of wind (*u* and *v*), potential temperature (θ), and turbulent kinetic energy (*e*) are provided by the prognostic fields in RAMS. This scheme is based on the prognostic equation for the turbulent kinetic energy which is solved in the meteorological model.

Define the turbulent kinetic energy (TKE), *e*, as:

$$e = 0.5\left(\overline{u'^2} + \overline{v'^2} + \overline{w'^2}\right) \tag{6}$$

Following is the prognostic equation for *e,* which is derived by manipulation of the Reynolds-averaged equations of motion:

$$\frac{\partial e}{\partial t} = -u_i \frac{\partial e}{\partial x_i} + \frac{\partial}{\partial x_i}\left(K_e \frac{\partial e}{\partial x_i} \right) + P_s + P_b + \varepsilon \tag{7}$$

where the first term on the right hand side is the resolved scale advection of TKE and the second term is the subgrid diffusion. The pressure correlation term has been assumed to be equal to zero by means of the anelastic approximation.

P_s is the shear production term:

$$P_s = \overline{u_j^{'} u_i^{'}} \left(\frac{\partial u_i}{\partial x_j} \right) \tag{8}$$

Most implementations of the MY scheme assume that it is an *anisotropic* diffusion scheme, meaning that the horizontal and vertical directions are treated differently. This assumption is only valid if the horizontal grid spacing is much larger than the vertical grid spacing. Therefore, if this assumption is made, as we do in RAMS for the MY scheme, we can neglect horizontal gradients in the shear production term and rewrite (8) as:

$$P_S = K_m \left[\left(\frac{\partial u}{\partial z} \right)^2 + \left(\frac{\partial v}{\partial z} \right)^2 \right] \tag{9}$$

For *isotropic* subgrid diffusion schemes, RAMS will use all nine components of the deformation tensor in the shear production term.

P_b is the buoyancy production term:

$$P_b = -\frac{g}{\theta_v} K_h \frac{\partial \theta_v}{\partial z} \tag{10}$$

The expression for the dissipation term, ε, is given by:

$$\varepsilon = a_e \frac{e^{3/2}}{l} \tag{11}$$

The vertical eddy diffusivities for momentum, heat, and TKE are computed by:

$$\begin{aligned} K_m &= S_m l\sqrt{2e} \\ K_h &= S_h l\sqrt{2e} \\ K_e &= S_e l\sqrt{2e} \end{aligned} \tag{12}$$

The wind and temperature enter these calculations in the form of non-dimensional vertical gradients:

$$\begin{aligned} G_u &= \frac{l}{\sqrt{2e}}\frac{\partial u}{\partial z} \\ G_v &= \frac{l}{\sqrt{2e}}\frac{\partial v}{\partial z} \\ G_m &= G_u^2 + G_v^2 \\ G_h &= -\frac{g}{\theta}\frac{l^2}{e}\frac{\partial \theta}{\partial z} \end{aligned} \tag{13}$$

The turbulent length scale, *l*, is assumed after Mellor and Yamada (1982):

$$\begin{aligned} l &= \frac{\kappa(z+z_0)}{1+\kappa(z+z_0)/l_\infty} \\ l_\infty &= 0.1\frac{\int_0^H z\sqrt{e}dz}{\int_0^H \sqrt{e}dz} \end{aligned} \tag{14}$$

where κ is the Von Karman constant and z_0 is the roughness length.

An upper limit for *l* in stable conditions proposed by André et al. (1978) is given by:

$$l \le 0.75\left[\frac{e}{\left(\frac{g}{\theta}\frac{\partial \theta}{\partial z}\right)}\right]^{1/2} \tag{15}$$

The above condition implies the constraint: $G_h \ge -0.75^2$.

In the level 2.5 scheme, the functions S_m and S_h (non-dimensional eddy diffusivities) depend on non-dimensional gradients of wind and potential temperature:

$$S_m = \frac{A_1\{1-3C_1-3A_2[B_2(1-3C_1)-12A_1C_1-3A_2]G_h\}}{1-3A_2(7A_1+B_2)G_h+27A_1A_2^2(4A_1+B_2)G_h^2+6A_1^2[1-3A_2(B_2-3A_2)G_h]G_m} \quad (16)$$

$$S_h = A_2\frac{1-6A_1S_mG_m}{1-3A_2(4A_1+B_2)G_h} \quad (17)$$

Empirical constants are assigned values following Mellor and Yamada (1982):

$$\{A_1, A_2, B_1, B_2, C_1, S_e, a_e\} = \{0.92, 0.74, 16.6, 10.1, 0.08, 0.20, 2^{2/3}/16.6\} \quad (18)$$

Summary of MM5 TKE schemes

There are three TKE-based PBL schemes implemented in MM5:
1) Burk-Thompson (1989) (hereinafter, BT)
2) ETA (Janjic, 1990, 1994)
3) Gayno-Seaman (Shafran, et.al., 2000) (herinafter, GS)

All three of these schemes are based on the previous Mellor-Yamada work and are similar in many aspects. The main differences lie in the particular assumptions used in the computation of the scale length, the dissipation term, and the interface with the core model. The following sections will summarize the schemes.

Burk-Thompson scheme

The BT scheme was originally developed for inclusion in the Navy's NORAPS model in the late 1980's, when the regular model grid had a horizontal grid spacing of 80 km and only contained 10 layers. The work of Burk and Thompson involved creating a "nested" grid on which to compute the physical parameterizations. In the original work, the physics grid was expanded to 20 layers. They developed both a level 2.5 and a level 3.0 scheme, although only the level 2.5 is implemented in MM5. Additionally, BT did significant work with various subgrid moisture fluxes and a countergradient temperature term that were not implemented in MM5.

The BT scheme follows rather closely from the standard MY scheme in the computation of TKE, scale length, and the dissipation term. It is the only scheme in MM5 to use the

Louis (1979) surface layer parameterization, an empirical fit to the Businger profile functions. However, several approximations have made upon the scheme's implementation in MM5.

As also in Burk and Thompson (1989), horizontal and vertical advection of TKE have not been included. While horizontal advection becomes less important for the grid spacings that BT were concerned with, vertical advection is an important process. Horizontal diffusion of TKE is also not included.

The BT scheme only works with its own two layer, force-restore soil model. It does not interface to any of the MM5 soil models or land use schemes.

ETA scheme

The ETA TKE scheme follows very closely from the MY scheme, hence is very similar to the RAMS scheme described above. The surface layer fluxes are determined from an iterative scheme based on Mellor and Yamada (1982).

In the implementation in MM5, horizontal and vertical advection and horizontal diffusion are ignored. The scheme interfaces with the 5-layer soil model or the NOAH LSM.

Gayno-Seaman scheme

The GS scheme is the most recent TKE-based scheme, and most complete, that is included in MM5. One of the more unique features of the scheme is the use of liquid water potential temperature (Betts, 1973) as the temperature variable which is diffused, which is a more conservative quantity in a saturated atmosphere than temperature or potential temperature. This is also somewhat similar to RAMS where an ice-liquid water potential temperature is used as the prognostic quantity in all numerical processes.

The GS scheme also contains separate conceptual models for fog formation, dissipation, and subgrid condensation following the work of Bougeault (1981) and includes a countergradient term in the subgrid heat fluxes following the work of Therry and Lacarrere (1983). The heat flux term is then written as:

$$w'\theta_L' = -K_h\left(\frac{\partial \theta_L}{\partial z} - \gamma_g\right)$$

where the countergradient term γ_g is based on the surface sensible heat flux, boundary layer height, and the convective vertical velocity scale. The boundary layer height is determined as the level where the TKE reaches a small value (0.2 $m^2 s^{-2}$).

The length scales and the dissipation term are based on the work described in Ballard, et.al. (1991) for their implementation of a TKE scheme for the UK Met Office Mesoscale Model.

This is the only TKE scheme in MM5 that advects TKE itself and includes both horizontal and vertical advection. It also includes the horizontal diffusion of TKE.

The surface layer fluxes are determined by the same scheme as is used in the Blackadar PBL scheme (Grell, et.al., 1995). The surface layer momentum, heat, and moisture fluxes are determined by a bulk-aerodynamic based scheme from Deardorff (1972) which computes drag coefficients to determine the rate of transfer of the surface properties.

The GS implementation in MM5 will only work with the Blackadar slab soil model, the 5-layer soil, or the Pleim-Xiu scheme (not in MPI mode). It currently does not interface with the NOAH LSM.

Discussion and recommendations

All three of the MM5 TKE schemes are derived from the same work by Mellor and Yamada; hence there are numerous similarities in the basic philosophy of the schemes. They are based on a prognostic equation for TKE which, in combination with a scale length, specifies an eddy viscosity coefficient to be used in a standard second order diffusion term. The mixing of the atmospheric fields is done locally, although various non-local effects are included in the computation of the eddy viscosity coefficients.

However, when considering the details of the implementations of the schemes, the differences become rather striking. Some of the differences are based on the closure approximations for the scale length computation and the dissipation term. Some of the differences are comprised of features attempting to include additional effects not accounted for by MY, such as the use of liquid water potential temperature and the countergradient term by GS. But the main complicating factor in attempting to compare and evaluate these schemes in MM5 is the significant differences in how the individual schemes are implemented.

Because of the rather complicated expressions for eddy viscosity coefficient (e.g., Eq. 12, 16, and 17), it would be difficult, but not impossible, to analytically compare the formulations. But any conclusion based on this type of analysis would be overshadowed by the implementation differences. Any meaningful comparison of the existing schemes would need to account for these differences also. Following is a summary of the major differences and some of the difficulties in making accurate comparisons:

- Use of LSM/soil models – the BT scheme can only use its own force-restore soil model, which cannot be used by GS or ETA. ETA can use the NOAH LSM, but GS cannot. Therefore, in an actual case study, the comparison is limited to using the 5-layer soil with GS and ETA. There isn't a way to include the BT scheme at all and there isn't a way to use the more sophisticated NOAH LSM in a side-by-side comparison in a real case study.

- Advection and horizontal diffusion – the GS scheme includes the advection and horizontal diffusion terms. It can be argued that, on larger grid spacings, these terms are not important. However, these schemes are being used on rather high-resolution grids. In complex topography, there is significant advection of TKE from the tops of ridges that form neutral layers overlaying stable air in the valleys and plains. In sea breeze situations, the return flow advects turbulence above the marine air to help maintain an elevated, well-mixed layer. Using higher resolution grids, it would be difficult to compare the GS scheme to the ETA or BT because of the differences in these terms.

- Surface layer schemes – the fluxes from the surface layer provide the lower boundary conditions for the actual PBL diffusion. A surface layer scheme computes these fluxes based on information from the soil/vegetation/water characteristics and (usually) the lowest layer atmospheric variables. Each of the MM5 TKE schemes uses a different surface layer scheme; BT uses a Louis scheme, GS uses a Deardorff scheme, and the ETA scheme uses the scheme from MY. Within the surface layer scheme are various assumptions that can control, for example, the rate at which heat and moisture is given to the atmosphere. This process is self-correcting to an extent. For example, if the sensible heat flux is lower in one scheme, the ground will stay warmer. The next timestep will then compute a higher sensible heat flux. However, there can be time lags in reaching the high and low temperatures, and comparing TKE production terms can show significant differences.

Several questions can be raised:
1) Are the TKE schemes worth using if MM5's implementations are so inconsistent?
2) If the answer is yes, how can we structure experiments that can provide adequate information to compare the schemes?
3) What modifications should be made to the schemes to improve their performance (i.e., to remove the low PBL height bias) and improve surface verifications?

For the reasons stated in the Introduction, we feel that the answer to the first question is yes. The TKE schemes provide a much more scientifically-defensible alternative to the profile schemes such as the MRF. And since other models use TKE schemes with success, the likelihood is that the technology can be included in MM5 in an attempt to improve some of the wind, temperature, moisture biases that we and others have noted consistently in the MM5 results.

Following is our recommendation for a work plan to investigate and improve the TKE schemes in MM5:

- The Burk-Thompson scheme should be dropped from consideration. It was developed for rather coarse horizontal and vertical grid spacing and implemented in the least complete way in MM5. Many of the more sophisticated features from the original BT work are not included in the MM5 implementation.
- Configure idealized scenarios to compare the ETA and GS schemes. The MRF scheme could be included for comparison also. One possibility is to set up the model in a horizontally-homogeneous configuration, as we did for the idealized tests in ATMET (2003a), then run a several hour experiment where the surface layer fluxes are specified. This removes the degrees of freedom of the surface model and the surface layer schemes. TKE, eddy diffusivities, and boundary layer structure can be compared and evaluated.
- With this idealized configuration, it would be possible to implement the RAMS MY scheme as an additional basis of comparison.
- Our expectation, based on previous experience, is that the MRF will develop the fastest growing and highest PBL height, the RAMS MY scheme will be next, followed by the ETA, and lastly the GS. However, if the TKE and K profiles are similar in these tests among the schemes, then we know that the differences in the surface layer and soil models are the underlying causes of the overall model differences.
- By following this process of systematically adding back in the degrees of freedom (and striving for consistency in the implementation of the schemes), we can determine what aspect of the entire process in causing the most differences and which can be improved. An attractive by-product is that we can implement, for example, an interface of the GS scheme to the NOAH LSM. It may also be possible to have a complete implementation of the RAMS MY scheme in MM5.

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